Phosphoramidic acid, dimethyl-, dimethyl ester

597-07-9	DTXSID20208405	

Model Performance

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 5.46e-01 mmHg

Global applicability domain: Inside

Local applicability domain index: 5.96e-01

Confidence level: 8.45e-01

Nearest Neighbors from the Training Set

Image not found

1,2-Phenylenediamine **Measured:** 4.14e-01

Predicted: 8.53e-04

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1,3-Diethenylbenzene

Measured: 9.00e-01 Predicted: 8.63e-01

Image not found

4-Bromophenol

Measured: 4.10e-01 Predicted: 2.33e-02

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4,4'-Bipyridine

Measured: 1.14 Predicted: 5.62e-05

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Acetic acid, chloro-, 1-methylethyl

ester

Measured: 2.69e-01 Predicted: 6.23